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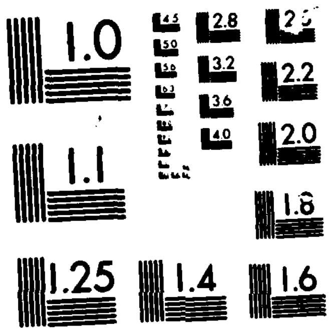

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NAVAL POSTGRADUATE SCHOOL

Monterey, California

DIFFUSION ESTIMATES HANDBOOK
(APPLICATION TO THE SPACE SHUTTLE
HCl EXHAUST CLOUD)

by

G. E. SCHACHER, S. LARSEN, and T. MIKKELSEN

FEBRUARY 1986

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Prepared for: US Air Force, Space Division
Los Angeles, CA 90009

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A simplified method is presented for making atmospheric diffusion estimates. The method is applied to the Space Shuttle HCl exhaust hazard at Vandenberg Air Force Base. A set of standard parameters and results are developed and applications to specific areas are included.

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I. Introduction

The purpose of this report is to present a simplified means for making approximate estimates of the far field impact of HCl from the Space Shuttle exhaust cloud. The two principle reasons for doing this are: 1) to make available a calculation methodology that can be easily used by anyone interested in the problem and 2) to establish baseline estimates of the HCl concentration which can be used here to determine the effects of varying critical model parameters.

The philosophy of the approach used here is that the first thing needed in hazard assessment is a gross estimate. If the estimate shows that the hazard is 100 times less than the target threshold (say a federal health standard), the hazard is insignificant and the problem is finished. If the estimate shows a hazard 100 times the threshold, corrective actions must be taken. Often the estimate is somewhere within an order of magnitude of the threshold and it is necessary to improve the estimation methodology before conclusions can be drawn. Initially, the quality of the approach need only be good enough to insure accuracy within the needed gross estimate range.

The problem under consideration here is diffusion in the complex terrain at Vandenberg Air Force Base. This problem is much too difficult to be adequately handled by any currently available model. The only diffusion calculations that can be used for the area can give, at best, order of magnitude concentration estimates. It is not practical to try to make

accurate calculations until an adequate model for the area is available. Thus, the estimation procedure presented here is not only a good first step but the appropriate approach to use at this time. Apparently accurate calculations may be misleading in that they obscure uncertainties in the results and could lead to incorrect operational decisions.

As was stated above, the approach presented here treats the far field hazard. It does not deal with the near field rainout problem. The best available information on that effect is the operational REEDM model.

The far field hazard will be due to both gaseous HCl and to acidic aerosols. We do not know the balance between these two components, only an estimate of the total HCl in the cloud, so we treat HCl as a single entity. The physiological response to the two components may be quite different and separating them may be important to the final results. Physiological response are not a consideration in this report. This is a clear inadequacy, but such information is not available.

The assumptions made in the calculations are clearly outlined in what follows. In the last section we describe ways we expect to relax some of these assumptions and make improvements in the estimations.

This report is laid out in the following way: First we describe the most simplified version of the model we use, the box model. The more complicated Gaussian model is discussed in an appendix. We then describe the initial cloud, which yields needed input information for the model. Next, sets of standard

parameters, methodologies, and results are developed. This section acts as a guide to anyone wishing to use these methods, and the results can be used directly to make diffusion estimates if one wishes. The estimated impact on specific areas is determined next, with both on-base and off-base areas treated. Finally, we compare our results to the operational REEDM model.

As much as possible, we make the sections dealing with diffusion results self contained. Thus, the reader can utilize sections IV and V without little reference to the rest of the report.

II. The Model

The model has one set of simplifying assumptions and two calculation methodologies, box and Gaussian. The only difference in the two methods is that they use slightly different horizontal HCl mass distributions. The simplifying assumptions are:

1. The cloud has uniform concentration in the vertical from the surface up to the mixing depth.

2. The mixing depth is defined by the inversion height.

3. Gaseous and aerosol components may be lumped together into a single concentration estimate.

4. Deposition can be calculated from a rate which is contant over the plume travel time.

5. The characteristics of the initial cloud, when stabilized, are well known and may be used as a model input.

6. The air trajectory distance from the source to the impact point may be used to calculate the cloud size.

The affect these assumptions have on the accuracy of the calculations are well within the desired accuracy of the results. Also, the assumptions can be easily modified to produce more accurate estimates when appropriate (when we know how to do so).

We will illustrate how results produced with these assumptions compare to a much more complicated model toward the end of this report.

Box Model

We describe the box approach first for the sake of simplicity, then the Gaussian approach will be a modification to it. Gaussian results are included in this section but derived in an Appendix. After the near-field rainout has occured, the total amount of HCl left in the cloud is (source strength)

$$\text{Initial HCl} = M.$$

This material is spread uniformly over a volume defined by

$$\text{Initial width} = \Delta x_o = \Delta y_o$$

$$\text{Initial Depth} - \Delta z.$$

The values used for these parameters will be described in the next section.

As the cloud moves with the mean wind, diffusion will increase the dimensions of the cloud to Δx, Δy, and Δz. There is no limit to Δx and Δy but vertical growth is constrained by the inversion height Z_i. We assume the cloud is well mixed in the vertical, so

$$\Delta z = Z_i \tag{1}$$

We assume that $\Delta x = \Delta y = \Delta$ and that they can be determined from the Pasquill curves[1] shown in Figure 1. For the near-neutral conditions most often encountered at Vandenberg, the plot shows that

$$\Delta(R) = 2\sigma \simeq 2(R/20) \tag{2}$$

where R is the downwind range. The relation between Δ and σ will be described later. Note that the Pasquill curves were obtained from experiments on flat plain and do not accurately apply to the complex terrain at Vandenberg. Their use is within the accuracy

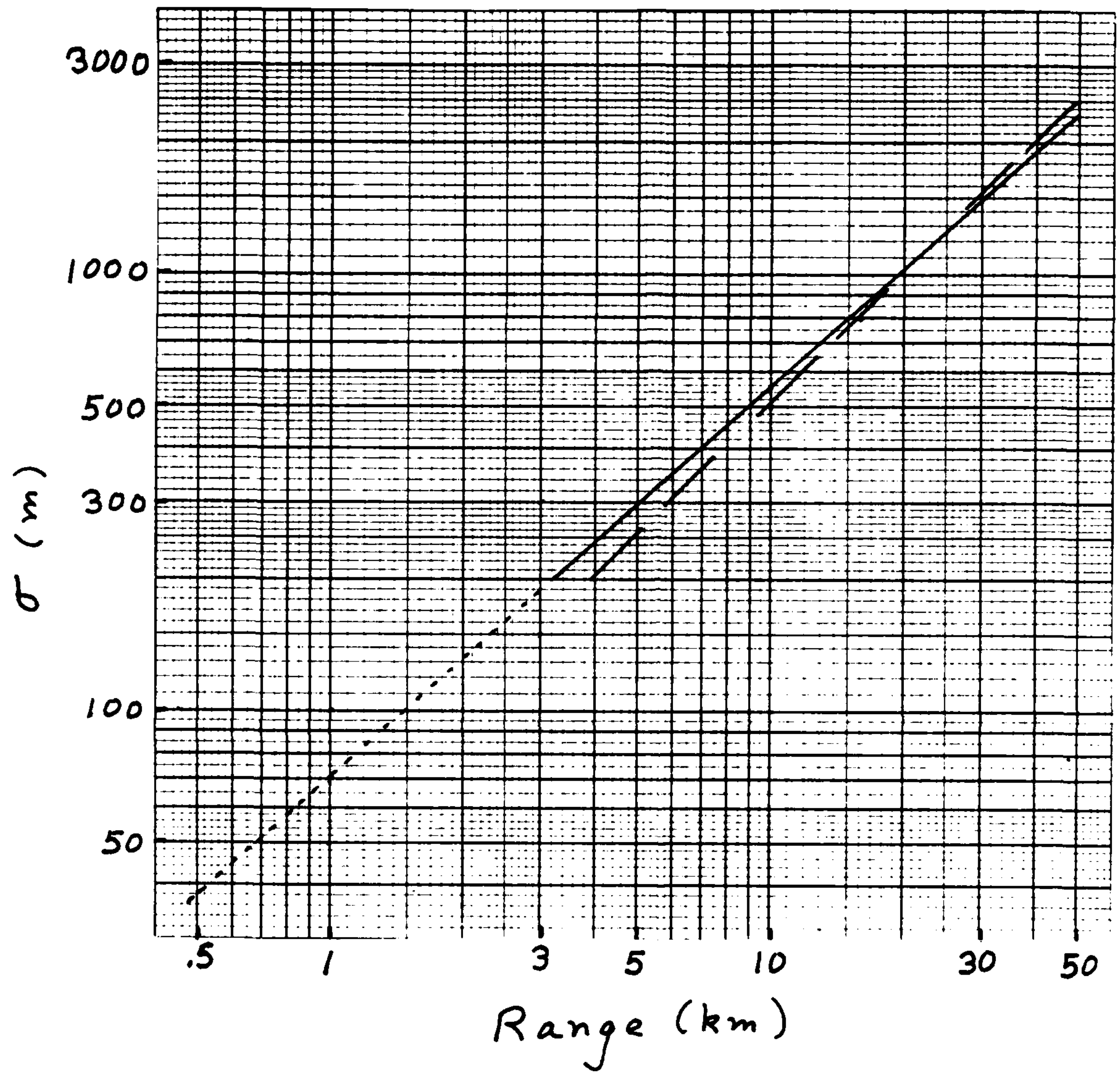


Figure 1. Horizontal dispersion standard deviation as a function of downwind range (neutral stability). Solid line is the standard result, dotted extension is beyond limit of applicability. Dashed line is the R/20 approximation.

of the approximate method being developed here. Figure 1 shows the difference between the real curve and the R/10 approximation. The difference is small in the region of validity for this model. The method is not applicable for cloud sizes less than 200m, the initial cloud size. The dotted line indicates this region. The dashed line is the R/10 approximation.

Instantaneous Concentration

The instantaneous concentration at range R from the source is simply

$$\chi(R) = \frac{M}{Z_i \Delta(R)^2} \tag{3}$$

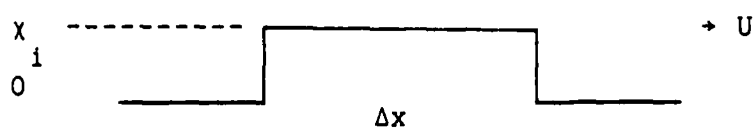
If the range is short, it may be that $\Delta(R)$ is less than Δx_o. In that case, it is not appropriate to use $\Delta(R)$ and the initial size of the cloud must be known. (The initial concentration must be used). This is given by

$$\chi_o = \frac{M}{\Delta x_o \Delta y_o Z_i} \tag{4}$$

Values for these parameters are given in the section on the initial properties of the cloud.

Time Average Concentration

For many health standards, it is necessary to determine the average concentration over some averaging time. Refering to the following drawing



the cloud of length Δx and constant instantaneous concentration χ_i is moving past a point with speed U. We let

$$T = \text{averaging time}$$

and the transit time is

$$\tau = \Delta x/U. \tag{5}$$

If the transit time is greater than the averaging time, the time average and instantaneous concentrations will be the same.

$$\chi_T = \chi_i \qquad T > \tau \tag{6}$$

If the averaging time is the larger, the average concentration will be reduced due to the cloud being present for only a fraction of the time:

$$\chi_T = \chi_i\left(\frac{\tau}{T}\right). \qquad T > \tau \tag{7}$$

Substituting Eqns 3 and 5 into 7 and recognizing that $\Delta x = \Delta(R)$ we have

$$\chi_T = \frac{1}{T}\,\frac{M}{UZ_i\Delta(R)} \qquad T > \tau \tag{8}$$

Note that in the far field, the initial cloud parameters do not enter into χ_i or χ_T and that the downwind extent of the cloud is not a factor in the time average concentration unless the averaging time is shorter than the time for cloud passage.

As was stated above, the Gaussian results are derived in Appendix B. We write both these and the box model results below for ease of reference. The symbols have been slightly simplified and are described in Appendix A. We write the Gaussian results as simple modifications of the box.

Instantaneous Concentration:

Box: $\chi_i = M/\Delta^2 Z_i$ (9)

Gaussian: $\chi_i^G = (2/\pi)\chi_i$ (10)

Time Average Concentration:

Box: $\chi_T = (\tau/T)\chi_i$ $\tau<T$ (11)

$= M/TU\Delta Z_i$ (12)

Gaussian: $\chi_T^G = \sqrt{2/\pi}A(T/\tau)\chi_T$ (13)

Concentration Threshold Size and Impact Time:

Gaussian: $\delta x = \Delta\sqrt{2\ln(\chi_i/\chi_{th})}$ (14)

$\delta t = \delta x/U$

Illustrations of the use of these equations are presented in Section IV

III. Initial Cloud

The Space Shuttle launch situation is very complicated as far as determining the configuration and concentration of the initial cloud. We will make no attempt to describe nor predict the properties of the initial cloud. Rather, we will make use of what information is available to us from analysis of previous launches. This information was developed for Kennedy and may need significant modification for the Vandenberg situation. The information we have comes from three sources: REEDM users manual[2], an analysis of cloud rainout[3], and Aerospace Corporation[4]. We present the parameters we use and some other parameters that we don't need, such as velocities and accelerations, so that our assumed properties can be checked when more information becomes available.

During the launch phase, the main motors fire, there is a time delay, then the boosters fire and the shuttle is released. We count time from the release point. As the shuttle rises, the exhaust rate is relatively constant, so that the mass of HCl released per unit height continually decreases as the velocity increases. The height, velocity, total mass released and mass/height, as functions of time, are presented in Table 1. Figures 1 and 2 show these data graphically.

t(sec)	h(ft)/(m)	v(m/sec)	$M(10^3 kg)$	h(m)	$M(10^3 kg)$	C(kg/m)
0	193/59	0	0	0	0	0
2	215/66	0.6	9.58	200	41	205
4	300/91	15.3	20.3	400	64	113
6	453/138	24.6	31.1	600	78	73
7	559/170	29.6	36.6	800	91	63
8	679/207	34.4	42.1	1000	102	55
10	962/293	44.0	53.2	1200	112	50
12	1385/422	55.7	64.4	1400	121	48
14	1831/558	66.2	75.6	1600	130	43
16	2381/726	77.4	86.8			
18	3014/919	88.7	98.1			
20	3732/1137	100.3	109.4			
22	4539/1383	112.0	120.6			
24	5431/1655	123.8	131.7			

Table 1. Shuttle parameters as functions of time which were used to calculate inital HCl cloud properties. C is the mass released per meter in the previous 200 meters.

In the calculations presented in this report, we do not use the vertical mass distribution shown in Table 1. Rather, we assume the total mass released up to the inversion height is distributed uniformly. We also assume the horizontal size of the cloud is 200m. Thus

$$\Delta z_o = Z_i$$

$$\Delta x_o = \Delta y_o = 200m$$

Using these values, Equation 4, and Table 1, we calculate the following values of total mass and HCl concentration for various inversion heights:

Z_i(m)	M(10^3kg)	X_o(g/m^3)	X_o(ppm)
200	41	5.1	4200
300	54	4.5	3700
500	71	3.6	3000
700	84	3.0	2500
1000	102	2.6	2100

Table 2. HCl total mass released and concentration as functions of inversion height.

Since federal health standards are specified in parts per million mass ratio, in Table 2 we have included concentration in those units, as well as the conventional kg/m^3. The conversion factor is

$$1 \text{ mg/m}^3 = 0.82 \text{ ppm}$$

A significant fraction of the HCl exhausted will be rained out due to the deluge water (lower most portion of the cloud) and due to water vapor condensation by the hydroscopic HCl. We will not consider this loss mechanism at this point. It will be used as a parameter in the next section.

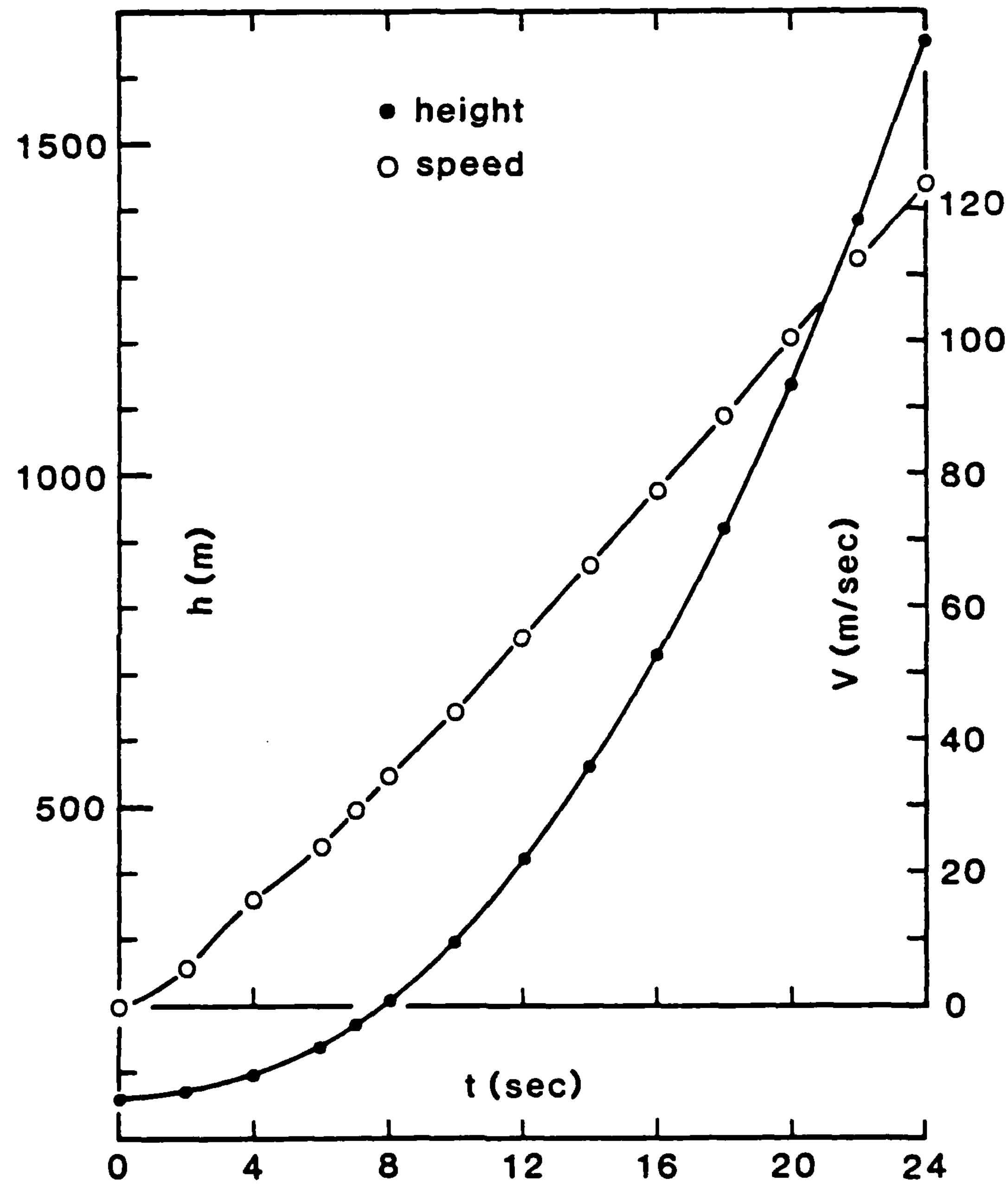


Figure 2. Shuttle height and speed as functions of time

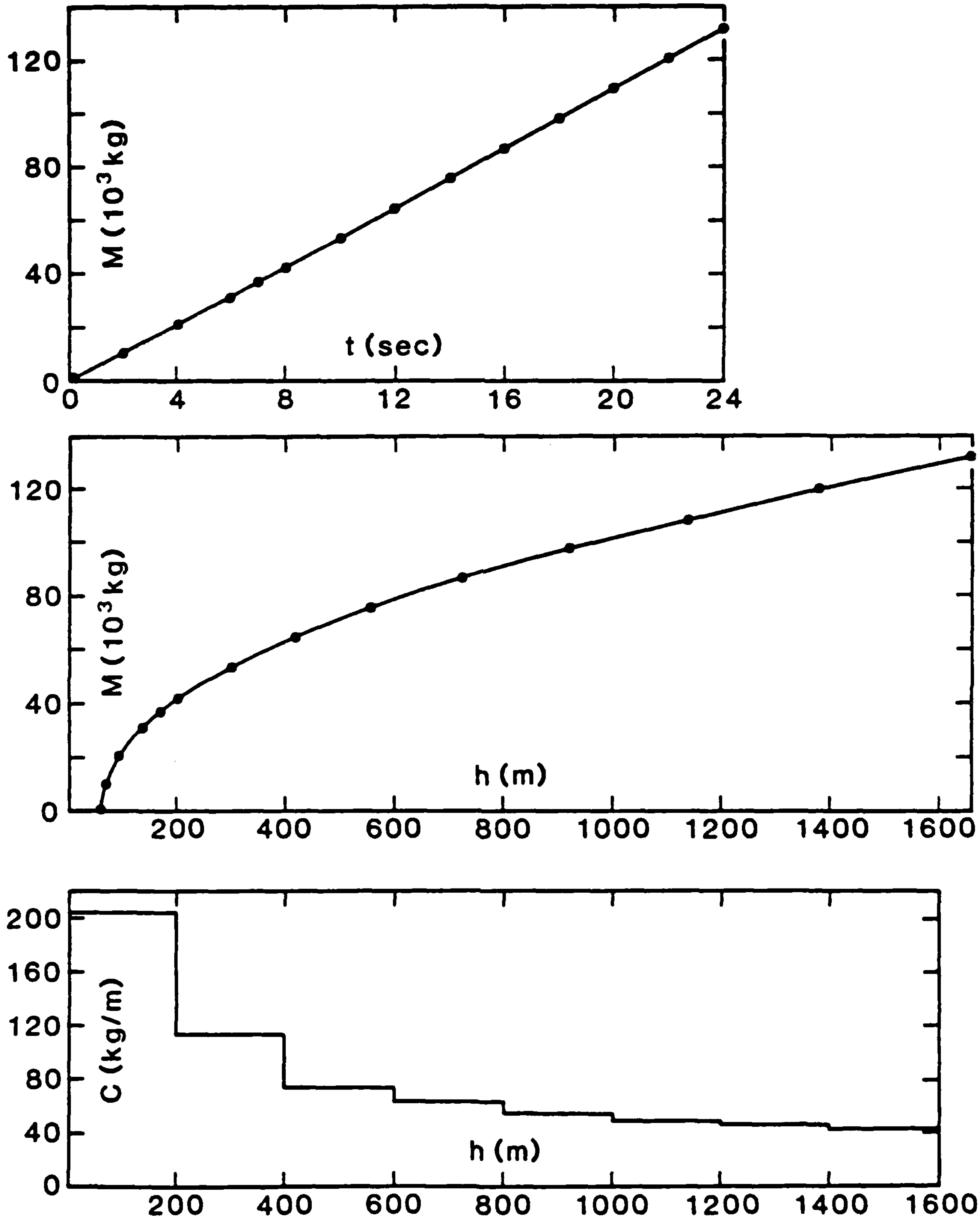


Figure 3. Shuttle HCl exhaust properties: total mass versus time, total mass versus height, and mass/length versus height

IV. Standard Parameters and Results

The purpose of this section is to establish a set of parameters and results that can be easily used by various people working on the Shuttle exhaust problem. The parameters will be standard and remain constant, the results will not. We expect to modify the results as our modeling capabilities improve.

The values we will use for the various input parameters are

Wind Speed	U	= 2, 5, 10 m/sec
Downwind Range	R	= 4, 8, 18, 30 km
Inversion Height	Z_i	= 200, 300, 500, 700, 1000 m
Averaging Time	T	= 10 min (600 sec)
Initial Cloud Size	Δ_o	= 200 m
Rainout Loss	L	= 0, ½
Deposition Rate	D	= dM/dR (unknown)
Threshold Concentration	χ_{th}	= 5ppm

The inversion height and initial cloud size determine the properties of the initial cloud. These were presented in Section III and are repeated here.

Z_i(m):	200	300	500	700	1000
M(10^6g) :	41	54	71	84	102
χ_o(g/m^3):	5.1	4.5	3.6	3.0	2.6

We will further simplify our former equations by noting that, if we assume $\Delta = R/10$, we can write for the box model,

$$\chi_i = 4\chi_o/R^2(\text{km}), \qquad \Delta = R/10 \tag{15}$$

$$\chi_T = 400\chi_o/UTR(km), \tag{16}$$

where R is now in km. This gives an extremely easy means for obtaining results from χ_o or converting results for various ranges, wind speeds, etc.

If one wishes results based on the Gaussian model, they can be obtained from the following simple conversions:

$$\chi_i^G = 2\chi_i/\pi \tag{17}$$

$$\chi_T^G = \sqrt{2/\pi}\,[A(T/\tau)]\chi_T \tag{18}$$

The standard results will be for the following parameters

$$U = 5 \text{ m/sec}$$

$$R = 8 \text{ km}$$

$$Z_i = 500 \text{ m}$$

$$L = \tfrac{1}{2}$$

$$D = 0$$

We now present, step by step, the way these parameters are used to obtain the desired results:

1) From $\Delta = R/10$ and $\sigma = \Delta/2$

$\Delta = 800$ M,

$\sigma = 400$ M.

2) From $\tau = \Delta/U$, $\sigma_T = \sigma/U$, and Table B-1 with $f = T/\tau$

$\tau = 160$ sec,

$\sigma_T = 80$ sec,

$A(f) = 1.0$.

3) From Table 2, Z_i = 500 m, and reducing χ_o by a factor of 2 for L = ½

$$M = 7.1X10^7 \text{ g},$$

$$\chi_o = 3.6 \text{ g/m}^3.$$

4) From Equations 15 and 16 (use R in km)

$$\chi_i = 112 \text{ mg/m}^3 \quad (92 \text{ ppm}),$$

$$\chi_T = 30 \text{ mg/m}^3 \quad (24 \text{ ppm}).$$

5) From Equations 17 and 18

$$\chi_i^G = 71 \text{ mg/m}^3 \quad (58 \text{ ppm}),$$

$$\chi_T^G = 19 \text{ mg/m}^3 \quad (16 \text{ ppm}).$$

6) From Equations B-12 and B-13 and using a 5 ppm threshold

$$\delta x = 414 \text{ m}$$

$$\delta t = 83 \text{ sec}$$

Using the method described above we have calculated the various concentrations for all of the standard parameters. For ease of reference, we present those results here. Note that only the box concentration, χ_i, is presented since everything else is easily derived from it from Equations 15-18.

If one wishes to save time and effort, one can use the two tables of results, interpolate for different parameters if needed, or use the equations presented in this section to obtain concentration results for any set of parameters.

$\chi_i (mg/m^3)$

for Z_i =

R(km)	200m	300m	500m	700m	1000m
4	632	560	448	376	320
8	158	140	112	94	80
16	40	36	28	24	20
30	12	10	8.0	6.6	3.6

Table 3. Box model concentration for various ranges and inversion heights.

δt (sec)

for Z_i =

R(km)	200m	300m	500m	700m	1000m
4	230	230	220	220	210
8	380	370	355	340	330
16	540	520	570	430	390
30	400	180	-	-	-

Table 4. Exposure times for concentration exceeding 5 ppm for various ranges and inversion heights. Windspeed U = 5 m/sec. When no entries appear the concentration never reaches 5 ppm.

V. Impact on Specific Hazard Areas

In this section we examine the impact of the Space Shuttle HCl cloud on specific areas that may be considered sensitive. We make use of the results in the former section rather than going through detailed calculations over again. We also briefly discuss the meaning of the results.

For all of these results we assume the following parameters

$$Z_i = 500 \text{ m}$$

$$U = 5 \text{ m/sec} \quad (10 \text{ kts})$$

$$L = \tfrac{1}{2}$$

$$D = 0$$

We pick a 50% rainout loss because this is approximately the value measured at Kennedy. We will discuss deposition in the last section; the value $D = 0$ is reasonable.

For the areas we choose to examine, the parameters, and results are presented in the following table.

	Lompoc	Titan Site	Ridge Line	Ridge Line Indirect	Jalama Public Beach	Ocean Beach
R (km)	16	6	3	7	15	12
Δ (m)	1600	600	300	700	1500	1200
τ (sec)	320	120	60	140	300	240
χ_i (ppm)	23	163	654	120	26	41
χ_T (ppm)	12	33	65	28	13	16
χ_i^G (ppm)	15	104	416	76	17	26
χ_T^G (ppm)	8	21	42	18	8	10
δ_T (sec)	570	290	180	330	550	440

Table 5. Model results for specific hazard areas. The results are presented in parts per million so that comparisons with health standards can be easily made.

It is obvious from the above results and those in Section IV that by far the greatest reduction in HCl concentration comes from increased distance from the source. The other parameters are only secondary perturbations compared to distance.

The federal health standards for HCl are not completely clear. 5ppm is the maximum allowed, with 2 ppm as the threshold for one-half hour (?) or longer averages. We will consider only

5 ppm "never to exceed".

Based on this criterion, the standard is considerably exceeded at all sites. We expect the Gaussian model results to be more accurate than the box and comparison with the standard should be made with this value.

Taking Lompoc as an example, the 5 ppm standard is exceeded in the following way.

instantaneous concentration = 3 x standard

standard exceeded for 9 ½ min

The results are roughly the same for Jalama beach, which is outside the base to the southeast, and Ocean beach which is between North and South Vandenberg.

At the Titan site, the concentration is much higher. However, due to the small size of the cloud, the impact time will be approximately one-half the Lompoc value (290 vs 570 sec).

The on-base sites contain a considerable amount of delicate electronics equipment. HCl can damage electronic components at concentrations which are less than the human health standards. No standards for this hazard have been set so we cannot address that problem here.

The ridge line refers to the ridge behind the shuttle site which contains a number of installations. We include two sets of results for the ridge. The first is a direct cloud trajectory which would only occur with a West wind, an unusual occurrence. The other case is an "indirect" trajectory, a situation that has been observed in the Vandenberg wind records. Wind from the North or Northwest can move the cloud to the South of Pt Arguello then a change in wind direction can bring it back ashore and up the ridge line from the South. The distance used for this scenario is only an estimate. The ridge line concentration is high for either path, especially high for the direct path because the distance is so small.

IV. Comparison with REEDM Model

The REEDM model is installed at both Kennedy and Vandenberg, is operational at Kennedy and undergoing tests at Vandenberg. We have available to us the NASA Contractor Report 3646, which is the model user's manual. The manual was developed for the Kennedy version and may not be completely appropriate for the comparisons presented here.

In order to make a valid comparison, we must make sure that REEDM and we use the same total amount of HCl as a model input. Using the data on pages 9 and 10 of the users manual, they report the rate at which HCl is released as

$$\begin{aligned} \text{REEDM HCl rate} &= (\text{fuel expenditures}) \times (\text{HCl fraction}), \\ &= (1.5219 \times 10^7) \times (0.1146), \\ &= 1.74 \times 10^6 \text{ g/sec.} \end{aligned}$$

The data we present in Table 1 gives

$$\text{Correct HCl rate} = 5.36 \times 10^6 \text{ g/sec.}$$

The ratio of these rates is 3.1, which must be taken into account in our comparisons. The reason for the discrepancy is probably the change to high performance boosters for STS-8.

The following comparisons are made with the REEDM run for 12 Nov 1981, found on page A-6 of the report. For their data

$$\begin{aligned} U &- 8 \text{ m/sec} \\ Z_i &= 1047 \text{ m} \\ &- 1000 \text{ m} \end{aligned}$$

We interpret their first layer height of 1047 m to be the inversion height but this is not necessarily the case. Their results are

R(km)	χ_i(ppm)	χ_T(ppm)	Arrival Time (min)	Departure Time (min)	Δt sec)
5	0.027	.001	2.85	9.64	407
8	0.783	0.102	7.82	15.60	467
10	0.901	0.123	11.13	19.57	506
16	0.571	0.080	21.04	31.50	628

Table 6. REEDM model results

For these same conditions, our Gaussian model results are

R(km)	χ_i(ppm)	χ_T(ppm)	τ(sec)	δt(sec)
5	108	11	63	156
8	42	7.0	100	206
10	27	5.6	125	230
16	10	3.3	200	235

Table 7. Gaussian model results for comparison to REEDM results.

Obviously, there is considerable disagreement between the two sets of results, even when you multiply the REEDM results by the factor of 3.1 to account for the greater exhaust rate. We believe that the main reason for the discrepancy is that the REEDM model has a cloud stabilization height of about 1500 m, and assumes low concentration at ground level. Our model assumes a well mixed cloud, so the ground level impact will be high.

We are not sure what the Δt from the REEDM model is, but suspect that it is the time interval for any detectable HCl. This would explain their large values compared to our τ and δt, which are for considerably higher HCl levels.

Which model is correct? The only way to answer that question is to know how well the exhaust cloud is trapped by the inversion. Obviously, we assume that the cloud will not rise above the inversion, will be well mixed by turbulence in the boundary layer, and that ground level concentrations will be high. There is a fair amount of evidence that this will be the case with the strong inversions that are present at Vandenberg.

It is important that considerable effort be expended to measure the far field cloud properties for the first few launches at Vandenberg to clear up disagreements in model assumptions.

We must reemphasize that this comparison is made to the Kennedy version of the REEDM model. The results for the Vandenberg version may be different. We will make comparisons to the new version results as soon as they become available.

VII. Possible Improvements to the Model

One of the main purposes of the NPS/Riso/Iowa State project is to produce a continued updating of diffusion calculations, with this report being only the first step. Most of this effort will go into improving determination of the cloud size, Δ or σ. We will not outline the work that will be done here, that is available in other documents.

Cloud size We now use $\Delta = R/10$ or Figure 1 to find the cloud size. We know that this formulation is a gross approximation that needs changing. In fact, it may well be that the parameterization should depend on the specific air trajectory (cloud growth depends on the terrian over which the cloud moves). We will soon change this simplified parameterization.

Rainout At this point in time, we have no information on how much of the HCl will be lost to near-field rainout at Vandenberg. Measurements at Kennedy indicate that about one-half of the HCl is lost in this manner. This result comes from measurement of the rainout, no good quantitative measurement has been made of the concentration in the far-field cloud. Of course, the situation at Vandenberg is different and the fraction rained out may be different.

When the Vandenberg measurements become available, the rainout fraction can be changed. Note that we are now using a 50% loss and we do not expect a major change in this value. Even

a substantial change in the loss will not, by itself, change the conclusions of this report but it certainly should be included in improvements to the model.

Deposition Deposition occurs due to interaction of the lower portions of the cloud with the surface. Pictures of the Kennedy cloud show that it is elevated so that deposition will be very small initially. As of this time we expect that deposition will not be important except for extreme meteorological conditions. A more complete discussion on this point can be found in Appendix C.

Stability When the atmosphere is stable, turbulence is suppressed, when unstable it is enhanced by thermal convections. Thus, one would expect that cloud growth, which is caused by turbulence, would be greater during unstable conditions. We assume neutral conditions in this report, which is the normal condition for a marine atmosphere. The cloud growth parameterization shown in Figure 1 is for neutral conditions; the full set of curves developed by Pasquill, Gifford, and Turner for stable to unstable conditions, show growth varying by as much as a factor of 8. This is an important effect which must be included at some point. However, we know the Pasquill curves are not correct for complex terrain so we postpone considering stability effects until a better turbulence parameterization is available.

Source Strength We have no assurance that the HCl exhaust rate from the Shuttle will always be the same, and inaccuracies in our value are possible. Correcting for a new exhaust rate is simple; change the source term in Section III.

Vertical Mass Distribution We have assumed a uniform vertical distribution of HCl. Figure 3 shows that the initial cloud has much greater concentration at lower elevations, ignoring cloud rise. Figure 3 certainly does not portray the vertical mass distribution, but it will not be uniform as we assume here. This effect should be included in future improvements, but it will lead to a more complicated approach.

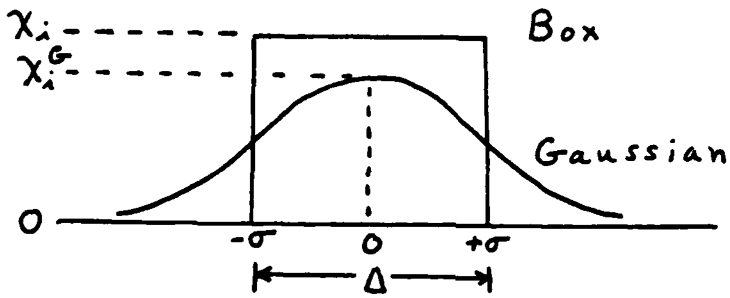
Appendix A. Symbols Used

The following are the simplified symbols used in this report. Where appropriate, the non-simplified symbols are also indicated.

Δ_o	Initial horizontal cloud size (Δx_o, Δy_o)
Δz_o	Initial cloud depth
Δ	Cloud horizontal size ($\Delta(R)$)
Z_i	Cloud depth (inversion height)
σ	Gaussian standard deviation ($\sigma = \Delta/2$)
R	Range
T	Averaging Time
U	Wind speed
τ	Cloud transit time ($\tau = \Delta/U$)
σ_t	Time standard deviation ($\sigma_t = \tau/2$)
f	Fraction of standard deviation ($f = T/2\sigma_t$)
A(f)	Gaussian integral
M	Total HCl mass
χ_o	Initial concentration
χ_i	Instantaneous concentration
χ_T	Time average concentration (superscript G for Gaussian)
χ_{th}	Threshold concentration (normally 5 ppm)
δx	Threshold cloud size
δt	Threshold impact time

Appendix B. Gaussian Model

Within the assumptions being used for this work, the only difference between the Gaussian and box approaches is the spatial horizontal distribution of the HCl. We assume the cloud uniformly fills the vertical up to Z_i for both approaches. The following drawing shows the way we distribute the HCl for both approaches.



We have set the horizontal size of the box equal to 2 times the Gaussian standard deviation. The standard deviation is the quantity plotted in Figure 1.

We require that the box and the Gaussian distribution contain the same amount of mass. Thus

$$\int_{-\infty}^{\infty} \chi(x,y,z)\, dxdydz = M \qquad \text{(B-1)}$$

For the Gaussian distribution

$$\chi^G = \frac{M}{2\pi\sigma^2 Z_i}\, e^{-x^2/2\sigma^2}\, e^{-y^2/\sigma^2} \qquad \text{(B-2)}$$

For the box

$$\chi = M/4\sigma^2 Z_i = X_i \qquad (x,y \text{ within } \Delta) \qquad \text{(B-3)}$$

Obviously, the instantaneous concentration at x = y = 0, the center of the Gaussian distribution, is

$$\chi_i^G = 2\chi_i/\pi \,. \tag{B-4}$$

Time Average Concentration

In order to obtain the time average concentration from the Gaussian distribution, it is necessary to integrate

$$\chi_T^G = \frac{1}{T} \int_{-T/2}^{T/2} \chi^G \, dt, \tag{B-5}$$

where the time integral would normally be centered on the time of passage of the center of the cloud. In order to most easily evaluate the integral, we write T in terms of σ and U:

$$U\frac{T}{2} = f\sigma, \tag{B-6}$$

where f is the fraction of the standard deviation that passes in time T/2 when the cloud is moving at speed U. We can write Eqn. B-5 as a Gaussian time intregral using x = Ut in Eqn B-2

$$\chi_T^G = \frac{1}{T} \chi_i^G \int_{-f\sigma_t}^{f\sigma t} e^{-t^2/2\sigma_T^2} \, dt, \tag{B-7}$$

where $$\sigma_t = \sigma/U = \tau/2. \tag{B-8}$$

Substituting $t = \sigma_t a$ gives

$$\chi_T^G = \frac{1}{T} \chi_i^G \sigma_T \int_{-f}^{f} e^{-a^2/2} da \qquad \text{(B-9)}$$

$$= (\sigma_t/T) \chi_i^G \sqrt{2\pi} A(f) \quad ,$$

where $f = (T/\tau) = (T/2\sigma_t)$. The Gaussian integral A(f) is related to the well known error function. For various fractions, it has the values given in Table B-1.

f	A(f)	f	A(f)	f	A(f)
0	0	1.0	.683	2.0	.954
0.1	.080	1.1	.729	2.1	.964
0.2	.159	1.2	.770	2.2	.972
0.3	.236	1.3	.806	2.3	.979
0.4	.311	1.4	.838	2.4	.984
0.5	.383	1.5	.866	2.5	.998
0.6	.451	1.6	.890	2.6	.991
0.7	.516	1.7	.901	2.7	.993
0.8	.576	1.8	.928	2.8	.995
0.9	.632	1.9	.942	2.9	.996

Table B-1. Gaussian integral (fraction of the total integral over the Gaussian distribution) as a function of the fraction of the standard deviation.

Thus, $$\chi_T^G = \sqrt{2\pi} \chi_i^G (\sigma_T/T) A(T/2\sigma_T) \qquad \text{(B-10)}$$

The values of χ_T^G/χ_i^G for various values of T/σ_T, are listed below for convenience.

T/σ_T:	0.1	0.5	1.0	2.0	3.0	5.0	7.0	10	20
χ_T/χ_i:	1.0	.99	.96	.86	.72	.50	.36	.25	.13
χ_T/χ_i:	1.0	1.0	1.0	1.0	.67	.50	.29	.20	.10

The ratio of the time average to the instantaneous concentration is also shown for the box model. The differences in the box and Gaussian ratios are insignificant. Recall that $\chi_i = 1.5\ \chi^G{}_i$, so the above does not imply that the two methods give the same concentrations.

Concentration Threshold

It may be of interest to calculate the size of the cloud that is above a given concentration threshold or the total time the concentration is above that threshold. This cannot be done with the box model since it assumes a constant concentration.

Using the Gaussian model, the concentration decreases from its peak value exponentially:

$$\left.\frac{\chi}{\chi_i}\right)_G = e^{-x^2/2\sigma^2} \quad . \tag{B-11}$$

Thus, the distance at which the concentration falls to the threshold value,

$$\delta x = 2\sigma\sqrt{2\ln(\chi_i^G/\chi_{th})} . \tag{B-12}$$

The impact time for the concentration at or above the threshold is simply

$$\delta t = \delta x/U \tag{B-13}$$

Appendix C. Deposition

Deposition is due to interaction of the lower portions of the cloud with the surface. The rate at which it occurs depends on the rate of transport to the surface, the interaction of the constituent with the surface, and the concentration near the surface. Transport to the surface is predominently by turbulence. The details of the interaction with the surface are seldom known, so this parameter and the transport rate are often lumped into a single parameter, the deposition velocity,

$$v_d = \text{deposition velocity.} \tag{C-1}$$

The rate of loss of mass in the cloud is

$$\frac{dM}{dt} = - \chi(0) v_d \Delta^2, \tag{C-2}$$

where $\chi(0)$ is the concentration at the surface. Since we assume the HCl is uniformly mixed in the vertical

$$\chi(0) = \chi = M/\Delta^2 Z_i. \tag{C-3}$$

Thus we have

$$\frac{dM}{dt} = - M v_d / Z_i. \tag{C-4}$$

We see that the loss rate does not depend on the horizontal size of the cloud, which is as expected since an increase in cloud size, and contact area with the ground, is compensated by reduced concentration.

Integrating and solving for M we have

$$M = M_o \exp(-v_d t/Z_i), \tag{C-5}$$

where M_o is the initial mass and t is the travel time. This can be rewritten in terms of the range and wind speed

$$t = R/U, \tag{C-6}$$

giving

$$M/M_o = \exp[-(R/Z_i)(v_d/U)]. \tag{C-7}$$

Equations C-7 is easy to use to find the fraction of the initial mass remaining in the cloud. Unfortunately, v_d is not known. Values of deposition velocity of 1-10 cm/sec would be quite high, so we will use those limits to assess the impact of deposition. Quick calculations yield the following results for a 10 km range and windspeed of 5 m/sec:

v_d(cm/sec)	Z_i(m)	M/M_o
1	1000	0.98
10	1000	0.82
1	200	0.90
10	200	0.37

Table C-1. Depositional reduction of mass in the HCl exhaust cloud, for R= 10 km and U = 5 m/sec.

Only for the extreme, and unrealistic, case of a very low inversion and an extremely high deposition rate does deposition have a significant effect on the HCl concentration. If the cloud is elevated during a portion of its trajectory, the total mass lost to deposition would be reduced. We conclude that deposition can be ignored at this time and can be reconsidered if more information becomes available after the first few Vandenberg Shuttle launches.

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